

# Alexander Sodt

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## CV

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### Education

Ph. D. in Chemistry *2007*  
University of California, Berkeley  
Thesis title: "Electronic structure on large molecules: Fast two-electron integrals and linear dependence"  
Advisor: Martin Head-Gordon

B.S. in Chemistry and Physics *2000*  
University of Washington, Seattle

### Post-doctoral work

Post-doctoral fellow  
Advisor: Richard W. Pastor, December 2009-present.  
Post-doctoral fellow  
Advisor: Teresa Head-Gordon, September 2007-October 2009.

### Teaching

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- **Teaching Assistant.** Chemistry 1A (twice), UC Berkeley
- **Teaching Assistant.** Quantitative Analysis, UC Berkeley

### Awards

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- **Hypercube Scholar**, University of Washington
- **Outstanding Basic Science Award 2013**, NHLBI/NIH

### Grants

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- **NIH/NHLBI K22 Career Development Grant**, 1-K22-HL121128-01 (2014)

### Publications

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1. A. J. Sodt, Y. Mei, G. König, P. Tao, R. P. Steele, B. R. Brooks, and Y. Shao, Multiple Environment Single System Quantum Mechanical/Molecular Mechanical (MESS QM/MM) Calculations. I. Estimation of Polarization Energies *J. Phys. Chem. A* , (*in press*)
2. B. S. Perrin Jr., A. J. Sodt, M. L. Cotten, and R. W. Pastor, The curvature induction of surface-bound antimicrobial peptides piscidin 1 and piscidin 3 varies with lipid chain length. *J. Membr. Biol.* (*in press*)
3. P. Tao, A. J. Sodt, Y. Shao, G. König, B. R. Brooks, Computing the free energy along a reaction coordinate using rigid body dynamics. *J. Chem. Theor. Comp.* **10**, 4198-4207 (2014)
4. R. M. Venable, A. J. Sodt, B. Rogaski, H. Rui, E. Hatcher, A. D. MacKerell Jr., R. W. Pastor, and J. B. Klauda, CHARMM all-atom additive force field for sphingomyelin: Elucidation of hydrogen bonding and positive curvature. *Biophys. J.* **107** 134-145 (2014)
5. A. J. Sodt and R. W. Pastor, Molecular modeling of lipid membrane curvature induction by a peptide: More than simply shape. *Biophys. J.* **106** 1958-1969 (2014)
6. A. J. Sodt, M. L. Sandar, K. Gawrisch, R. W. Pastor, and E. Lyman, The molecular structure of the liquid-ordered phase of lipid bilayers. *J. Am. Chem. Soc.* **136** 725-732 (2014)

7. A. J. Sodt and R. W. Pastor, Bending free energy from simulation: Correspondence of planar and inverse hexagonal lipid phases.  
*Biophys. J.* **104** 2202-2211 (2013)
8. L. Zhang, A. J. Sodt, R. M. Venable, R. W. Pastor and M. Buck, Prediction, Refinement and Persistency of Transmembrane Helix Dimers in Lipid Bilayers using Implicit and Explicit Solvent/Lipid Representations: Microsecond Molecular Dynamics Simulations of ErbB1/B2 and EphA1.  
*Proteins: Struct., Funct., Bioinf.* **81** 365-376 (2013)
9. A. J. Sodt and R. W. Pastor, The tension of a curved surface from simulation.  
*J. Chem. Phys.* **137** 234101 (2012)
10. C. M. Pfefferkorn, F. Heinrich, A. J. Sodt, A. S. Maltsev, A. S., R. W. Pastor, and J. C. Lee, Depth of  $\alpha$ -Synuclein in a Bilayer Determined by Fluorescence, Neutron Reflectometry, and Computation.  
*Biophys. J.* **102** 613-621 (2012)
11. J. Subotnik, J. Vura-Weis, A. J. Sodt and M. Ratner, Predicting accurate electronic excitation transfer rates via Marcus theory with Boys or Edmiston-Ruedenberg localization diabatization.  
*Journal of Physical Chemistry, A.* **114** 8665-8675 (2010)
12. A. J. Sodt and T. Head-Gordon, An implicit solvent coarse-grained lipid model with correct stress profile.  
*Journal of Chemical Physics* **132** 205103 (2010)
13. A. J. Sodt and T. Head-Gordon, Driving forces for transmembrane alpha-helix oligomerization.  
*Biophysical Journal* **99** 227-237 (2010)
14. A. J. Sodt and M. Head-Gordon, Hartree-Fock exchanged computed using the atomic resolution of the identity approximation.  
*Journal of Chemical Physics* **128** 104106 (2008)
15. J. Subotnik, A. J. Sodt and M. Head-Gordon, The limits of local correlation theory: Electronic delocalization and chemically smooth potential energy surfaces.  
*Journal of Chemical Physics* **128** 034103 (2008)
16. J. Subotnik, A. J. Sodt and M. Head-Gordon, Localized orbital theory and ammonia triborane.  
*Physical Chemistry Chemical Physics* **9** 5522-5530 (2007)
17. A. J. Sodt, J. Subotnik and M. Head-Gordon, Linear scaling density fitting.  
*Journal of Chemical Physics* **125** 194109 (2006)
18. J. Subotnik, A. J. Sodt and M. Head-Gordon, A near linear-scaling smooth local coupled cluster algorithm for electronic structure.  
*Journal of Chemical Physics* **125** 074116 (2006)
19. A. J. Sodt, G. Beran, Y. Jung and M. Head-Gordon, A fast implementation of perfect pairing and imperfect pairing using the resolution of the identity approximation.  
*Journal of Chemical Theory and Computation* **2** 300-305 (2006)
20. G. Beran, B. Austin, A. J. Sodt and M. Head-Gordon, Unrestricted perfect pairing: The simplest wave-function-based model chemistry beyond mean field.  
*Journal of Physical Chemistry A* **109** 9183-9192 (2005)
21. Y. Jung, A. J. Sodt, P. Gill, and M. Head-Gordon, Auxiliary basis expansions for large-scale electronic structure calculations.  
*Proc. Natl. Acad. Sci. U.S.A.* **102** 6692-6697 (2005)

## Invited talks

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1. “Spontaneous curvature from simulation”, Workshop: Physics, Chemistry and Biology of Membrane Proteins, Arizona State University (2012),
2. “Mechanical properties of peptide-membrane systems”, Workshop: Advances in Biomolecular Simulations in CHARMM, (2012) ,
3. “Modeling how membrane mechanical properties couple to protein function”, Kansas University, Center for Bioinformatics, April 2013
4. “Quantitative molecular modeling of lipid membrane curvature induction”, University of Delaware, Chemistry, Oct 2013
5. “Methods and model systems for computing membrane curvature free energies”, International Workshop on Biomembranes, Espoo, Finland (2014)